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1,3-Di-*o*-tolylthiourea

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.105
Data-to-parameter ratio = 15.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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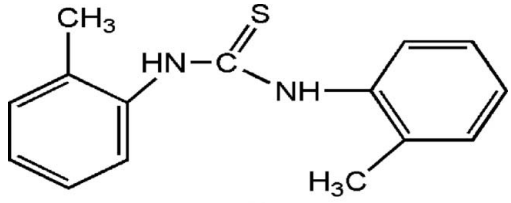
The two *o*-tolyl groups in the title compound, $C_{15}H_{16}N_2S$, are *trans* with respect to the thiourea unit. The asymmetric unit consists of two molecules linked by N—H···S hydrogen bonds into dimers.

Comment

The biological properties of thiourea complexes are well documented and thiourea derivatives have been successfully screened for various biological activities (Frech *et al.*, 1970). Thiourea derivatives are also useful ligands to a number of metals (König *et al.*, 1984; Schuster *et al.*, 1990). The molecular structure of the title thiourea derivative, (I), is reported here (Fig. 1).



(I)

There are two molecules in the asymmetric unit. The short C—S distances in (I) [1.6938 (16) and 1.6927 (16) Å] clearly shows double-bond character. For one molecule, the dihedral angles between the thiourea bridge and the C17- and C114-tolyl rings are 88.79 (8) and 61.05 (8)°, respectively, with the angle between the tolyl ring planes being 58.98 (8)°. The corresponding values for the second molecule are 87.61 (8), 79.61 (8) and 59.04 (8)°, respectively.

The two tolyl rings are mutually *trans* with respect to the N11—C115 or N21—C215 bonds of the thiourea units. This configuration favours dimer formation between the molecules (Ramnathan *et al.*, 1996) and, in this case, intermolecular N—H···S hydrogen bonds link the molecules into dimers (Fig. 2).

Experimental

A solution of *o*-toluidine (1.1 ml, 10 mmol) in acetone (20 ml) was added dropwise to a solution of CS_2 (0.90 ml, 10 mmol) and NH_3 (0.60 ml, 15 mmol) in acetone (50 ml). The mixture was stirred for about 4 h at room temperature and was then rotary-evaporated under vacuum. The crude product was added to 10% HCl (200 ml) and stirred well. The solid product was separated off and recrystallized from diethyl ether. The yield was 78%.

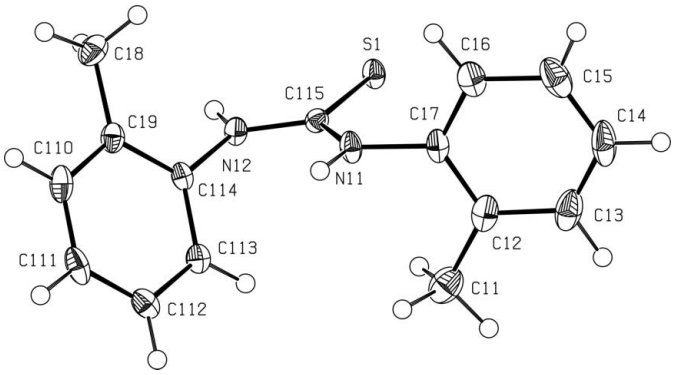


Figure 1
The structure of molecule 1 of the asymmetric unit. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

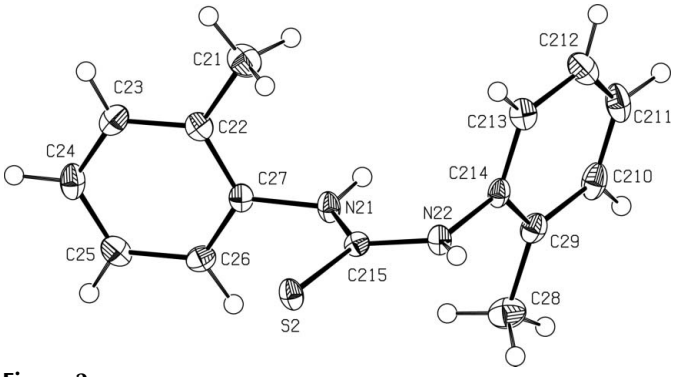


Figure 2
The structure of molecule 2 of the asymmetric unit. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

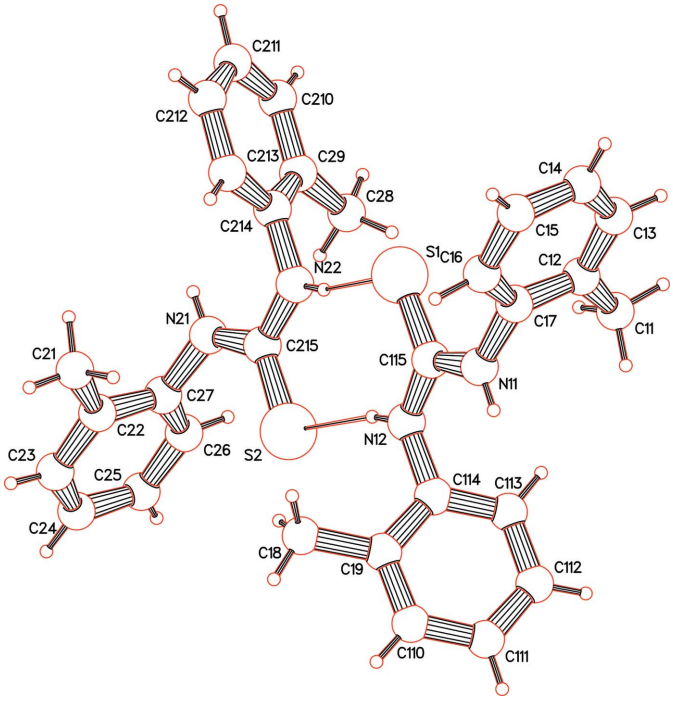


Figure 3
A perspective *PLUTO* (Meetsma, 2006) drawing of the dimer formed by N—H···S hydrogen bonds (narrow lines).

Crystal data

$C_{15}H_{16}N_2S$
M_r = 256.37
Monoclinic, $P2_1/n$
a = 12.3960 (9) Å
b = 9.5652 (7) Å
c = 23.163 (2) Å
β = 92.266 (1)°
V = 2744.3 (4) Å^3
Z = 8
D_x = 1.241 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 100 (1) K
Block, colourless
0.49 × 0.23 × 0.16 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.886, T_{max} = 0.966
22738 measured reflections
6776 independent reflections
5577 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 28.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.105
S = 1.05
6776 reflections
453 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0424P)^2 + 1.5124P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N12—H122···S2	0.87 (2)	2.49 (2)	3.3408 (14)	165.4 (18)
N22—H222···S1	0.87 (2)	2.43 (2)	3.2794 (14)	166.9 (17)

All H atoms were located in a difference Fourier map and were refined with isotropic displacement parameters [C—H = 0.92 (3)–1.03 (3) Å and N—H = 0.83 (2)–0.84 (2) Å].

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *DIRDIF99* (Beurskens *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLUTO* (Meetsma, 2006) and *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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supporting information

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Crystal data

$C_{15}H_{16}N_2S$
$M_r = 256.37$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 12.3960$ (9) Å
$b = 9.5652$ (7) Å
$c = 23.163$ (2) Å
$\beta = 92.266$ (1)°
$V = 2744.3$ (4) Å^3
$Z = 8$
$F(000) = 1088$

The final unit cell was obtained from the xyz centroids of 6808 reflections after integration using the SAINTPLUS software package (Bruker, 2000).
Reduced cell calculations did not indicate any higher metric lattice symmetry and examination of the final atomic coordinates of the structure did not yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)
$D_x = 1.241$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6808 reflections
$\theta = 2.3$–$29.1°$
$\mu = 0.22$ mm^{-1}
$T = 100$ K
Block, colourless
0.49 × 0.23 × 0.16 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine focus sealed Siemens Mo tube
Parallel mounted graphite monochromator
Detector resolution: 4096x4096/62x62 (binned 512) pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2000)

$T_{min} = 0.886$, $T_{max} = 0.966$
22738 measured reflections
6776 independent reflections
5577 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.7°$
$h = -16 \rightarrow 16$
$k = -12 \rightarrow 12$
$l = -30 \rightarrow 29$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.105$
$S = 1.05$
6776 reflections
453 parameters
0 restraints
Primary atom site location: heavy-atom method

Secondary atom site location: structure-invariant direct methods
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0424P)^2 + 1.5124P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.47963 (3)	0.74484 (4)	0.15212 (2)	0.0185 (1)
N11	0.64627 (11)	0.58167 (15)	0.12974 (6)	0.0195 (4)
N12	0.47770 (11)	0.48848 (14)	0.10861 (6)	0.0172 (4)
C11	0.71217 (17)	0.7660 (2)	0.04043 (9)	0.0329 (6)
C12	0.75265 (13)	0.78441 (18)	0.10166 (8)	0.0251 (5)
C13	0.82468 (15)	0.8907 (2)	0.11825 (10)	0.0332 (6)
C14	0.86198 (15)	0.9059 (2)	0.17500 (11)	0.0376 (7)
C15	0.82852 (15)	0.8145 (2)	0.21703 (10)	0.0354 (7)
C16	0.75686 (14)	0.7065 (2)	0.20185 (9)	0.0269 (5)
C17	0.71958 (12)	0.69366 (17)	0.14507 (8)	0.0206 (5)
C18	0.41792 (16)	0.2230 (2)	0.15657 (8)	0.0261 (6)
C19	0.48845 (13)	0.23336 (17)	0.10525 (7)	0.0191 (5)
C110	0.52634 (14)	0.11385 (18)	0.07810 (8)	0.0248 (5)
C111	0.58774 (14)	0.12300 (19)	0.02944 (8)	0.0262 (5)
C112	0.61274 (13)	0.25207 (19)	0.00640 (8)	0.0218 (5)
C113	0.57748 (13)	0.37261 (17)	0.03319 (7)	0.0182 (4)
C114	0.51644 (12)	0.36341 (16)	0.08239 (7)	0.0156 (4)
C115	0.53793 (12)	0.59647 (16)	0.12843 (7)	0.0157 (4)
H11	0.7434 (19)	0.841 (3)	0.0147 (10)	0.045 (7)*
H11′	0.7317 (19)	0.670 (3)	0.0261 (10)	0.050 (7)*
H11″	0.631 (2)	0.775 (2)	0.0386 (10)	0.045 (7)*
H13	0.8476 (17)	0.956 (2)	0.0878 (9)	0.035 (6)*
H14	0.9114 (18)	0.978 (2)	0.1856 (10)	0.042 (6)*
H15	0.8510 (18)	0.820 (2)	0.2553 (10)	0.036 (6)*
H16	0.7343 (13)	0.6321 (17)	0.2313 (7)	0.006 (4)*
H18	0.4460 (18)	0.276 (2)	0.1883 (10)	0.038 (6)*
H18′	0.4079 (18)	0.127 (3)	0.1680 (10)	0.044 (6)*
H18″	0.344 (2)	0.261 (2)	0.1473 (10)	0.046 (7)*
H110	0.5075 (16)	0.025 (2)	0.0937 (9)	0.029 (5)*
H111	0.6107 (17)	0.039 (2)	0.0118 (9)	0.035 (6)*
H112	0.6531 (16)	0.261 (2)	−0.0273 (9)	0.025 (5)*
H113	0.5935 (15)	0.463 (2)	0.0182 (8)	0.018 (5)*
H121	0.6717 (16)	0.506 (2)	0.1170 (8)	0.026 (5)*
H122	0.4078 (18)	0.497 (2)	0.1109 (9)	0.030 (5)*
S2	0.20838 (3)	0.48035 (4)	0.09584 (2)	0.0194 (1)
N21	0.04656 (11)	0.64940 (15)	0.12219 (6)	0.0189 (4)

N22	0.21681 (11)	0.74524 (14)	0.12945 (6)	0.0173 (4)
C21	0.00271 (17)	0.4945 (2)	0.22449 (8)	0.0285 (6)
C22	−0.04967 (13)	0.45726 (17)	0.16709 (7)	0.0187 (5)
C23	−0.12127 (14)	0.34519 (18)	0.16081 (8)	0.0223 (5)
C24	−0.16923 (13)	0.31106 (18)	0.10754 (8)	0.0232 (5)
C25	−0.14683 (13)	0.39005 (19)	0.05912 (8)	0.0226 (5)
C26	−0.07660 (13)	0.50254 (18)	0.06428 (7)	0.0191 (4)
C27	−0.02766 (12)	0.53382 (16)	0.11744 (7)	0.0168 (4)
C28	0.12245 (17)	0.9518 (2)	0.05150 (8)	0.0294 (6)
C29	0.13615 (13)	0.97793 (17)	0.11524 (7)	0.0201 (5)
C210	0.10626 (14)	1.10519 (18)	0.13975 (8)	0.0246 (5)
C211	0.11820 (14)	1.12838 (19)	0.19848 (9)	0.0268 (5)
C212	0.16143 (15)	1.0259 (2)	0.23491 (8)	0.0271 (5)
C213	0.19259 (14)	0.89874 (18)	0.21176 (8)	0.0219 (5)
C214	0.17978 (12)	0.87550 (16)	0.15252 (7)	0.0173 (4)
C215	0.15426 (12)	0.63346 (16)	0.11717 (7)	0.0156 (4)
H21	0.0813 (18)	0.483 (2)	0.2220 (9)	0.031 (5)*
H21′	−0.0161 (18)	0.592 (2)	0.2346 (9)	0.039 (6)*
H21″	−0.0213 (19)	0.436 (3)	0.2537 (11)	0.048 (7)*
H23	−0.1361 (16)	0.294 (2)	0.1947 (9)	0.028 (5)*
H24	−0.2176 (16)	0.233 (2)	0.1047 (8)	0.025 (5)*
H25	−0.1780 (15)	0.368 (2)	0.0229 (8)	0.022 (5)*
H26	−0.0607 (15)	0.561 (2)	0.0327 (8)	0.019 (5)*
H28	0.1000 (19)	1.042 (3)	0.0345 (10)	0.045 (6)*
H28′	0.191 (2)	0.927 (2)	0.0344 (10)	0.044 (6)*
H28″	0.072 (2)	0.874 (3)	0.0435 (10)	0.054 (7)*
H210	0.0801 (15)	1.179 (2)	0.1144 (8)	0.025 (5)*
H211	0.0980 (17)	1.218 (2)	0.2137 (9)	0.031 (5)*
H212	0.1672 (17)	1.040 (2)	0.2753 (10)	0.033 (6)*
H213	0.2218 (15)	0.826 (2)	0.2360 (8)	0.020 (5)*
H221	0.0255 (17)	0.722 (2)	0.1378 (9)	0.027 (5)*
H222	0.2861 (18)	0.732 (2)	0.1322 (9)	0.028 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0141 (2)	0.0142 (2)	0.0274 (2)	0.0011 (2)	0.0030 (2)	−0.0055 (2)
N11	0.0142 (7)	0.0135 (7)	0.0309 (8)	0.0013 (5)	0.0010 (5)	−0.0063 (6)
N12	0.0125 (7)	0.0141 (6)	0.0251 (7)	0.0008 (5)	0.0030 (5)	−0.0033 (5)
C11	0.0311 (11)	0.0268 (10)	0.0412 (12)	0.0026 (8)	0.0054 (9)	0.0078 (9)
C12	0.0151 (8)	0.0172 (8)	0.0433 (11)	0.0030 (6)	0.0056 (7)	−0.0027 (7)
C13	0.0192 (9)	0.0231 (9)	0.0579 (14)	−0.0026 (8)	0.0104 (9)	−0.0044 (9)
C14	0.0170 (9)	0.0274 (10)	0.0690 (15)	−0.0060 (8)	0.0076 (9)	−0.0195 (10)
C15	0.0212 (9)	0.0395 (12)	0.0453 (13)	0.0009 (8)	−0.0019 (8)	−0.0207 (10)
C16	0.0167 (8)	0.0266 (9)	0.0375 (10)	0.0014 (7)	0.0027 (7)	−0.0098 (8)
C17	0.0098 (7)	0.0160 (8)	0.0362 (10)	0.0009 (6)	0.0037 (6)	−0.0083 (7)
C18	0.0280 (10)	0.0235 (9)	0.0267 (10)	−0.0027 (8)	0.0012 (7)	0.0081 (7)
C19	0.0170 (8)	0.0172 (8)	0.0227 (8)	−0.0014 (6)	−0.0042 (6)	0.0012 (6)

C110	0.0239 (9)	0.0130 (8)	0.0370 (10)	−0.0007 (7)	−0.0046 (7)	−0.0002 (7)
C111	0.0214 (9)	0.0189 (9)	0.0379 (10)	0.0028 (7)	−0.0045 (7)	−0.0127 (7)
C112	0.0150 (8)	0.0264 (9)	0.0237 (9)	0.0021 (7)	−0.0021 (6)	−0.0076 (7)
C113	0.0141 (7)	0.0174 (8)	0.0229 (8)	0.0008 (6)	−0.0023 (6)	−0.0009 (6)
C114	0.0124 (7)	0.0136 (7)	0.0205 (8)	0.0016 (6)	−0.0033 (6)	−0.0029 (6)
C115	0.0162 (7)	0.0139 (7)	0.0172 (8)	0.0005 (6)	0.0021 (6)	0.0006 (6)
S2	0.0139 (2)	0.0152 (2)	0.0290 (2)	0.0023 (2)	0.0009 (2)	−0.0055 (2)
N21	0.0141 (7)	0.0131 (7)	0.0295 (8)	0.0010 (5)	0.0028 (5)	−0.0041 (6)
N22	0.0110 (6)	0.0142 (6)	0.0266 (7)	0.0020 (5)	0.0015 (5)	−0.0019 (5)
C21	0.0359 (11)	0.0261 (10)	0.0229 (9)	0.0043 (8)	−0.0061 (8)	0.0016 (7)
C22	0.0167 (8)	0.0173 (8)	0.0220 (8)	0.0050 (6)	0.0001 (6)	−0.0005 (6)
C23	0.0197 (8)	0.0191 (8)	0.0285 (9)	0.0036 (7)	0.0057 (7)	0.0051 (7)
C24	0.0134 (8)	0.0177 (8)	0.0386 (10)	−0.0002 (7)	0.0014 (7)	−0.0034 (7)
C25	0.0155 (8)	0.0273 (9)	0.0249 (9)	0.0022 (7)	−0.0014 (7)	−0.0072 (7)
C26	0.0142 (7)	0.0225 (8)	0.0208 (8)	0.0030 (6)	0.0039 (6)	0.0013 (7)
C27	0.0118 (7)	0.0152 (7)	0.0235 (8)	0.0017 (6)	0.0016 (6)	−0.0014 (6)
C28	0.0319 (10)	0.0313 (10)	0.0251 (10)	0.0074 (9)	0.0024 (8)	0.0062 (8)
C29	0.0140 (7)	0.0195 (8)	0.0271 (9)	0.0002 (6)	0.0033 (6)	0.0019 (7)
C210	0.0179 (8)	0.0157 (8)	0.0403 (11)	0.0008 (7)	0.0027 (7)	0.0037 (7)
C211	0.0187 (8)	0.0178 (8)	0.0440 (11)	−0.0001 (7)	0.0009 (7)	−0.0084 (8)
C212	0.0253 (9)	0.0274 (9)	0.0284 (10)	0.0004 (8)	−0.0002 (7)	−0.0093 (8)
C213	0.0193 (8)	0.0199 (8)	0.0264 (9)	0.0009 (7)	−0.0009 (7)	−0.0011 (7)
C214	0.0115 (7)	0.0139 (7)	0.0267 (9)	−0.0008 (6)	0.0038 (6)	−0.0009 (6)
C215	0.0156 (7)	0.0151 (7)	0.0162 (8)	0.0019 (6)	0.0007 (6)	0.0018 (6)

Geometric parameters (Å, º)

S1—C115	1.6938 (16)	C18—H18	0.95 (2)
S2—C215	1.6927 (16)	C18—H18′	0.97 (3)
N11—C115	1.350 (2)	C18—H18″	1.00 (2)
N11—C17	1.440 (2)	C110—H110	0.96 (2)
N12—C114	1.433 (2)	C111—H111	0.95 (2)
N12—C115	1.345 (2)	C112—H112	0.95 (2)
N11—H121	0.847 (19)	C113—H113	0.956 (19)
N12—H122	0.87 (2)	C21—C22	1.499 (2)
N21—C27	1.440 (2)	C22—C27	1.399 (2)
N21—C215	1.353 (2)	C22—C23	1.396 (2)
N22—C215	1.345 (2)	C23—C24	1.387 (3)
N22—C214	1.438 (2)	C24—C25	1.389 (3)
N21—H221	0.83 (2)	C25—C26	1.386 (2)
N22—H222	0.87 (2)	C26—C27	1.384 (2)
C11—C12	1.496 (3)	C28—C29	1.500 (2)
C12—C17	1.402 (2)	C29—C210	1.399 (2)
C12—C13	1.397 (3)	C29—C214	1.400 (2)
C13—C14	1.384 (3)	C21—H21	0.98 (2)
C14—C15	1.384 (3)	C21—H21′	0.99 (2)
C15—C16	1.398 (3)	C21—H21″	0.94 (3)
C16—C17	1.382 (3)	C23—H23	0.95 (2)

C18—C19	1.507 (3)	C24—H24	0.958 (19)
C19—C110	1.395 (2)	C25—H25	0.934 (19)
C19—C114	1.401 (2)	C26—H26	0.948 (19)
C110—C111	1.388 (3)	C28—H28′	0.98 (2)
C11—H11′	1.01 (3)	C28—H28″	0.99 (3)
C11—H11″	1.01 (2)	C28—H28	0.98 (3)
C111—C112	1.385 (3)	C210—C211	1.381 (3)
C11—H11	1.02 (3)	C211—C212	1.387 (3)
C112—C113	1.388 (2)	C212—C213	1.390 (3)
C113—C114	1.395 (2)	C213—C214	1.393 (2)
C13—H13	0.99 (2)	C210—H210	0.966 (19)
C14—H14	0.95 (2)	C211—H211	0.96 (2)
C15—H15	0.92 (2)	C212—H212	0.95 (2)
C16—H16	1.032 (16)	C213—H213	0.956 (19)

S1···N22	3.2794 (14)	C215···C28	3.420 (2)
S1···C12	3.6436 (17)	C210···H14^{vii}	2.94 (2)
S1···C16	3.5997 (18)	C211···H213^{ii}	3.094 (19)
S2···C26	3.5853 (17)	C211···H14^{vii}	2.94 (2)
S2···N12	3.3408 (14)	C214···H221	2.42 (2)
S2···C22	3.6636 (17)	C215···H21	2.99 (2)
S1···H110^{i}	3.03 (2)	C215···H28″	3.02 (3)
S1···H222	2.43 (2)	H11···H13	2.36 (3)
S1···H21″^{ii}	2.88 (3)	H11···H111^{i}	2.51 (3)
S1···H212^{iii}	3.20 (2)	H11···H28^{x}	2.55 (3)
S2···H18″	2.91 (2)	H11···C28^{x}	3.04 (3)
S2···H122	2.49 (2)	H11′···N11	2.79 (2)
S2···H25^{iv}	3.119 (19)	H11′···C26^{vi}	2.97 (3)
N11···C113	3.095 (2)	H11″···N11	2.81 (2)
N12···S2	3.3408 (14)	H11″···C115	2.96 (2)
N21···C29	3.339 (2)	H13···H11	2.36 (3)
N22···S1	3.2794 (14)	H14···C210^{vi}	2.94 (2)
N11···H113	2.874 (19)	H14···C211^{vi}	2.94 (2)
N11···H11′	2.79 (2)	H18···N12	2.78 (2)
N11···H11″	2.81 (2)	H18′···H110	2.37 (3)
N12···H18″	2.90 (2)	H18′···C21^{iii}	2.97 (2)
N12···H18	2.78 (2)	H18″···S2	2.91 (2)
N21···H21′	2.80 (2)	H18″···N12	2.90 (2)
N21···H28″	2.84 (3)	H18″···H122	2.55 (3)
N21···H21	2.83 (2)	H21···N21	2.83 (2)
N22···H28′	2.81 (2)	H21···C215	2.99 (2)
N22···H28″	2.90 (2)	H21···H211^{ix}	2.55 (3)
N22···H112^{v}	2.92 (2)	H21′···C16^{vii}	3.09 (2)
C11···C115	3.435 (3)	H21′···C18^{ii}	3.03 (2)
C12···S1	3.6436 (17)	H21′···N21	2.80 (2)
C12···C26^{vi}	3.556 (2)	H21′···C15^{vii}	2.89 (2)
C16···C22^{vi}	3.498 (2)	H21″···H23	2.36 (3)
C16···S1	3.5997 (18)	H21″···S1^{iii}	2.88 (3)

C17···C27^{vi}	3.567 (2)	H23···H21″	2.36 (3)
C21···C215	3.442 (3)	H23···C16^{iii}	2.99 (2)
C22···C16^{vii}	3.498 (2)	H24···C112^{vii}	3.043 (19)
C22···S2	3.6636 (17)	H25···H112^{vii}	2.57 (3)
C24···C112^{vii}	3.551 (2)	H25···C113^{vii}	3.050 (19)
C24···C113^{vii}	3.570 (2)	H25···C112^{vii}	2.833 (19)
C25···C112^{vii}	3.439 (2)	H25···S2^{iv}	3.119 (19)
C25···C113^{vii}	3.450 (2)	H26···C26^{iv}	2.935 (19)
C26···C12^{vii}	3.556 (2)	H26···H26^{iv}	2.47 (3)
C26···C26^{iv}	3.595 (2)	H28···H210	2.29 (3)
C26···S2	3.5853 (17)	H28···H11^{x}	2.55 (3)
C27···C17^{vii}	3.567 (2)	H28′···N22	2.81 (2)
C28···C215	3.420 (2)	H28″···N21	2.84 (3)
C29···N21	3.339 (2)	H28″···N22	2.90 (2)
C11···H111^{i}	2.96 (2)	H28″···C215	3.02 (3)
C111···C111^{viii}	3.449 (3)	H110···S1^{ix}	3.03 (2)
C112···C25^{vi}	3.439 (2)	H110···H18′	2.37 (3)
C112···C24^{vi}	3.551 (2)	H111···C11^{ix}	2.96 (2)
C113···C24^{vi}	3.570 (2)	H111···C111^{viii}	3.03 (2)
C113···C113^{v}	3.429 (2)	H111···H11^{ix}	2.51 (3)
C113···N11	3.095 (2)	H111···C110^{viii}	3.01 (2)
C113···C25^{vi}	3.450 (2)	H112···H25^{vi}	2.57 (3)
C13···H221^{vi}	2.99 (2)	H112···H222^{v}	2.57 (3)
C14···H221^{vi}	2.84 (2)	H112···N22^{v}	2.92 (2)
C115···C11	3.435 (3)	H113···N11	2.874 (19)
C15···H21′^{vi}	2.89 (2)	H113···H113^{v}	2.54 (3)
C16···H21′^{vi}	3.09 (2)	H113···C113^{v}	2.860 (19)
C16···H23^{ii}	2.99 (2)	H113···C115	2.960 (19)
C18···H21′^{iii}	3.03 (2)	H113···H121	2.48 (3)
C18···H122	2.827 (19)	H121···C24^{vi}	2.73 (2)
C21···H18′^{ii}	2.97 (2)	H121···C114	2.47 (2)
C21···H211^{ix}	2.91 (2)	H121···C25^{vi}	2.89 (2)
C21···H221	2.98 (2)	H121···C113	2.565 (19)
C22···H211^{ix}	3.10 (2)	H121···H113	2.48 (3)
C24···H121^{vii}	2.73 (2)	H122···H18″	2.55 (3)
C25···H121^{vii}	2.89 (2)	H122···S2	2.49 (2)
C26···H11′^{vii}	2.97 (3)	H122···C18	2.827 (19)
C26···H26^{iv}	2.935 (19)	H210···H28	2.29 (3)
C28···H11^{x}	3.04 (3)	H211···C21^{i}	2.91 (2)
C29···H221	2.86 (2)	H211···C22^{i}	3.10 (2)
C110···H111^{viii}	3.01 (2)	H211···H21^{i}	2.55 (3)
C111···H111^{viii}	3.03 (2)	H212···S1^{ii}	3.20 (2)
C112···H24^{vi}	3.043 (19)	H213···C211^{iii}	3.094 (19)
C112···H25^{vi}	2.833 (19)	H221···C13^{vii}	2.99 (2)
C113···H121	2.565 (19)	H221···C14^{vii}	2.84 (2)
C113···H25^{vi}	3.050 (19)	H221···C21	2.98 (2)
C113···H113^{v}	2.860 (19)	H221···C29	2.86 (2)
C114···H121	2.47 (2)	H221···C214	2.42 (2)

C115···H113	2.960 (19)	H222···S1	2.43 (2)
C115···H11″	2.96 (2)	H222···H112^{v}	2.57 (3)
C215···C21	3.442 (3)		

C17—N11—C115	123.04 (14)	C112—C111—H111	120.9 (13)
C114—N12—C115	126.52 (13)	C110—C111—H111	118.6 (13)
C17—N11—H121	118.8 (13)	C111—C112—H112	122.1 (12)
C115—N11—H121	117.7 (13)	C113—C112—H112	118.6 (12)
C114—N12—H122	117.0 (13)	C114—C113—H113	118.8 (11)
C115—N12—H122	116.5 (13)	C112—C113—H113	121.0 (11)
C27—N21—C215	122.45 (14)	C21—C22—C23	121.75 (15)
C214—N22—C215	125.29 (13)	C21—C22—C27	120.85 (15)
C27—N21—H221	117.7 (14)	C23—C22—C27	117.40 (15)
C215—N21—H221	117.4 (15)	C22—C23—C24	121.46 (16)
C215—N22—H222	117.4 (13)	C23—C24—C25	119.85 (16)
C214—N22—H222	115.4 (13)	C24—C25—C26	119.83 (16)
C11—C12—C17	120.70 (16)	C25—C26—C27	119.76 (15)
C11—C12—C13	122.23 (17)	N21—C27—C22	118.94 (14)
C13—C12—C17	117.08 (17)	N21—C27—C26	119.37 (14)
C12—C13—C14	121.58 (19)	C22—C27—C26	121.69 (15)
C13—C14—C15	120.24 (18)	C210—C29—C214	117.42 (15)
C14—C15—C16	119.7 (2)	C28—C29—C210	121.51 (15)
C15—C16—C17	119.35 (18)	C28—C29—C214	121.07 (15)
C12—C17—C16	122.09 (16)	C22—C21—H21″	111.1 (16)
N11—C17—C12	118.90 (16)	H21—C21—H21′	111.2 (17)
N11—C17—C16	118.99 (15)	C22—C21—H21′	109.6 (12)
C18—C19—C114	121.12 (15)	C22—C21—H21	108.5 (12)
C110—C19—C114	117.67 (15)	H21′—C21—H21″	108 (2)
C18—C19—C110	121.20 (15)	H21—C21—H21″	108.6 (19)
C19—C110—C111	121.32 (16)	C22—C23—H23	116.9 (12)
C110—C111—C112	120.50 (17)	C24—C23—H23	121.6 (12)
C12—C11—H11″	109.0 (13)	C25—C24—H24	120.9 (11)
H11—C11—H11″	108.5 (18)	C23—C24—H24	119.3 (11)
H11—C11—H11′	110 (2)	C24—C25—H25	120.9 (12)
C12—C11—H11	110.5 (14)	C26—C25—H25	119.3 (12)
H11′—C11—H11″	108.4 (18)	C25—C26—H26	122.7 (11)
C12—C11—H11′	110.1 (14)	C27—C26—H26	117.5 (11)
C111—C112—C113	119.27 (16)	H28—C28—H28′	106.6 (18)
C112—C113—C114	120.21 (15)	H28—C28—H28″	115 (2)
C14—C13—H13	121.0 (12)	H28′—C28—H28″	107.2 (19)
C12—C13—H13	117.4 (12)	C29—C28—H28	105.5 (14)
C19—C114—C113	121.00 (14)	C29—C28—H28′	111.8 (14)
N12—C114—C113	119.68 (14)	C29—C28—H28″	110.9 (14)
C15—C14—H14	119.1 (14)	C29—C210—C211	121.32 (16)
C13—C14—H14	120.7 (14)	C210—C211—C212	120.64 (17)
N12—C114—C19	119.27 (14)	C211—C212—C213	119.35 (17)
C14—C15—H15	123.6 (13)	C212—C213—C214	119.80 (16)
C16—C15—H15	116.7 (13)	N22—C214—C213	118.60 (14)

S1—C115—N11	121.17 (12)	C29—C214—C213	121.47 (15)
N11—C115—N12	117.76 (14)	N22—C214—C29	119.88 (14)
S1—C115—N12	121.07 (12)	N21—C215—N22	117.05 (14)
C15—C16—H16	122.0 (9)	S2—C215—N21	121.75 (12)
C17—C16—H16	118.6 (9)	S2—C215—N22	121.19 (12)
H18′—C18—H18″	106.1 (18)	C29—C210—H210	118.5 (11)
C19—C18—H18″	111.2 (13)	C211—C210—H210	120.1 (11)
C19—C18—H18′	111.4 (14)	C210—C211—H211	119.0 (12)
C19—C18—H18	111.7 (13)	C212—C211—H211	120.4 (12)
H18—C18—H18′	110.1 (19)	C211—C212—H212	120.9 (12)
H18—C18—H18″	106.1 (18)	C213—C212—H212	119.7 (12)
C19—C110—H110	117.8 (12)	C212—C213—H213	121.0 (11)
C111—C110—H110	120.9 (12)	C214—C213—H213	119.2 (11)

C115—N11—C17—C12	−88.0 (2)	C18—C19—C114—C113	−176.91 (15)
C115—N11—C17—C16	93.4 (2)	C110—C19—C114—C113	1.8 (2)
C17—N11—C115—S1	−6.9 (2)	C18—C19—C114—N12	0.4 (2)
C17—N11—C115—N12	174.27 (15)	C18—C19—C110—C111	177.41 (17)
C115—N12—C114—C19	125.25 (17)	C114—C19—C110—C111	−1.3 (3)
C115—N12—C114—C113	−57.4 (2)	C21—C22—C23—C24	−179.82 (17)
C114—N12—C115—S1	173.60 (12)	C27—C22—C23—C24	−0.3 (2)
C114—N12—C115—N11	−7.5 (2)	C21—C22—C27—N21	0.1 (2)
C215—N21—C27—C22	88.23 (19)	C21—C22—C27—C26	−178.88 (16)
C215—N21—C27—C26	−92.76 (19)	C23—C22—C27—N21	−179.46 (14)
C27—N21—C215—S2	8.5 (2)	C23—C22—C27—C26	1.5 (2)
C27—N21—C215—N22	−171.98 (14)	C22—C23—C24—C25	−0.5 (3)
C215—N22—C214—C29	−84.5 (2)	C23—C24—C25—C26	0.0 (3)
C215—N22—C214—C213	98.11 (19)	C24—C25—C26—C27	1.2 (2)
C214—N22—C215—S2	−174.39 (12)	C25—C26—C27—N21	178.96 (15)
C214—N22—C215—N21	6.1 (2)	C25—C26—C27—C22	−2.1 (2)
C17—C12—C13—C14	0.1 (3)	C28—C29—C210—C211	179.47 (17)
C11—C12—C17—N11	0.3 (2)	C214—C29—C210—C211	−0.7 (2)
C11—C12—C17—C16	178.93 (17)	C28—C29—C214—C213	−179.87 (16)
C13—C12—C17—N11	−179.33 (15)	C210—C29—C214—C213	0.3 (2)
C13—C12—C17—C16	−0.7 (2)	C28—C29—C214—N22	2.9 (2)
C11—C12—C13—C14	−179.58 (18)	C210—C29—C214—N22	−176.98 (14)
C12—C13—C14—C15	0.2 (3)	C29—C210—C211—C212	0.6 (3)
C13—C14—C15—C16	0.1 (3)	C210—C211—C212—C213	−0.2 (3)
C14—C15—C16—C17	−0.7 (3)	C211—C212—C213—C214	−0.2 (3)
C15—C16—C17—N11	179.66 (16)	C212—C213—C214—N22	177.46 (15)
C15—C16—C17—C12	1.0 (3)	C212—C213—C214—C29	0.2 (2)
C110—C19—C114—N12	179.10 (15)		

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) −*x*+1/2, *y*+1/2, −*z*+1/2; (iii) −*x*+1/2, *y*−1/2, −*z*+1/2; (iv) −*x*, −*y*+1, −*z*; (v) −*x*+1, −*y*+1, −*z*; (vi) *x*+1, *y*, *z*; (vii) *x*−1, *y*, *z*; (viii) −*x*+1, −*y*, −*z*; (ix) *x*, *y*−1, *z*; (x) −*x*+1, −*y*+2, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N12—H122···S2	0.87 (2)	2.49 (2)	3.3408 (14)	165.4 (18)
N22—H222···S1	0.87 (2)	2.43 (2)	3.2794 (14)	166.9 (17)